

INCOMPLETE MIXING AND REACTION IN HETEROGENEOUS POROUS MEDIA: A PARTICLE BASED NUMERICAL STUDY

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Reaction of dissolved substances in porous media is important in many applications relating to subsurface flows (e.g. anthropogenic contamination, development and assessment of remediation strategies, natural geochemical contamination).

In this study we focus on dissolved substances that react kinetically. In particular, we focus on the bimolecular reaction $A+B \rightarrow C$. When the substances are well mixed, as in batch experiments, the rate of an irreversible kinetic reaction $A+B \rightarrow C$ is denoted by K , and we can apply the thermodynamic law, e.g. $dC_A/dt = -KC_A C_B$. However, when the mixing is not complete, we encounter concentration segregation in the form of 'islands' of single species (either A or B in the above mentioned case), and the mixing between these 'islands' becomes a limiting factor to the reaction. Then the reaction slows down in comparison to the rate anticipated by the thermodynamic law.

Incomplete mixing is a phenomenon that can occur purely due to diffusive stochastic fluctuations in a system with a uniform or zero velocity field. However, a heterogeneous velocity field changes mixing phenomena as it gives rise to a competition between shearing action, which tends to tear solute plumes apart and diffusion, which tries to homogenize the system.

In this research we focus on mixing and reaction in heterogeneous flow fields in a 2D setting. The heterogeneous flow field can enhance the mixing and one expects to have a faster rate of reaction when compared to a homogenous flow field. This hypothesis is tested using a particle based numerical model (Benson & Meerschaert, 2008), simulating the flow, mixing and reaction in a rectangular domain with heterogeneous velocity fields. Ensemble average results over various simulations are used to evaluate the reaction rates. Finally, we will develop an accompanying theoretical approach to quantify and interpret incomplete mixing effects.

Key words: Eulerian and Lagrangian approaches for mixing quantification and reactive transport modeling, mixing models, kinetic reaction

References

Benson, D.A. and M. M. Meerschaert (2008), Simulation of chemical reaction via particle tracking: Diffusion-limited versus thermodynamic rate-limited regimes, *Water Resour. Res.*, 44, W12201, doi:10.1029/2008WR007111.